Scientific Computing Group

NCCS USERS MEETING

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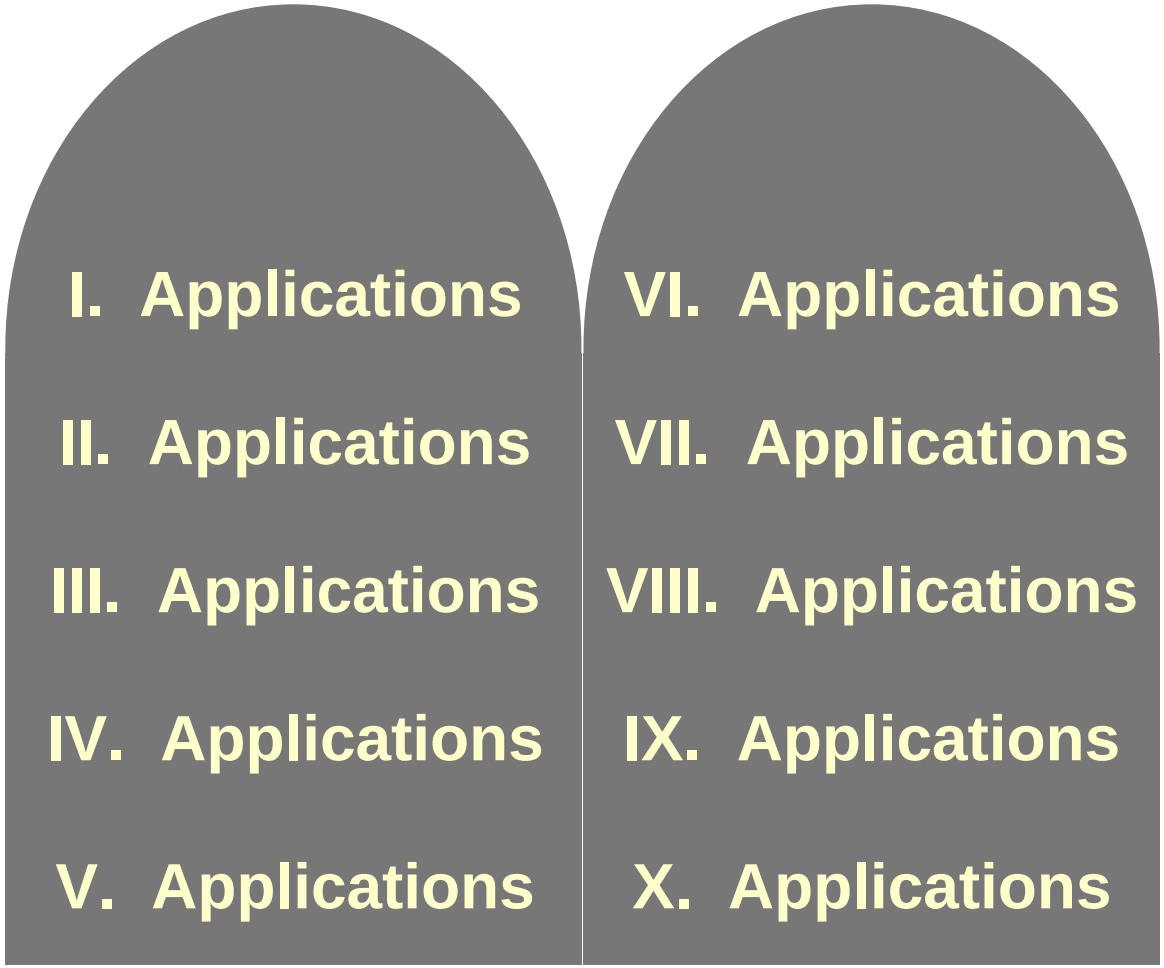
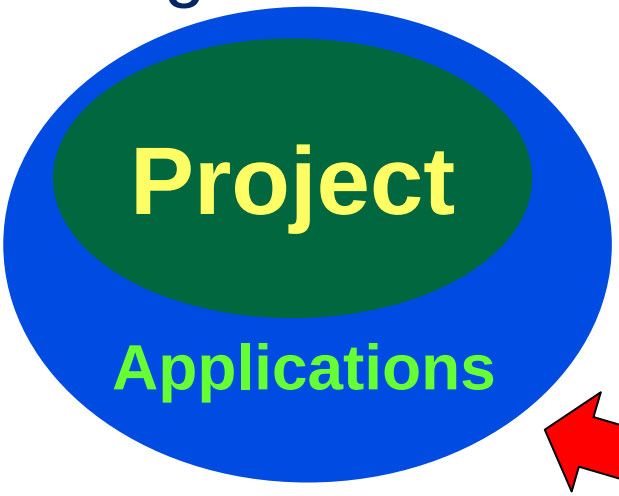
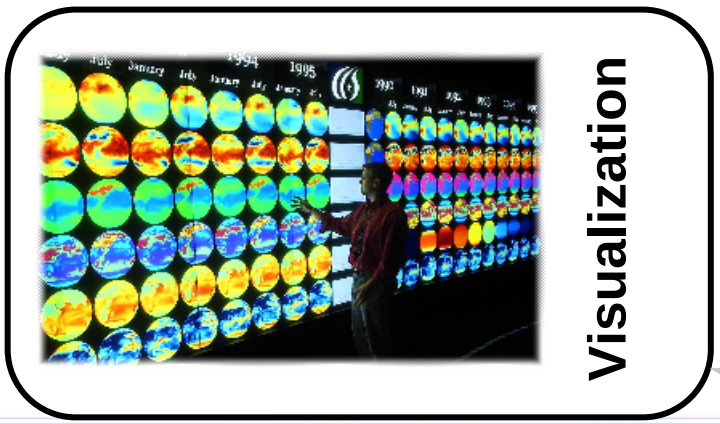
March 27, 2007

Ten Commandments for HPC



High-Level Consultation



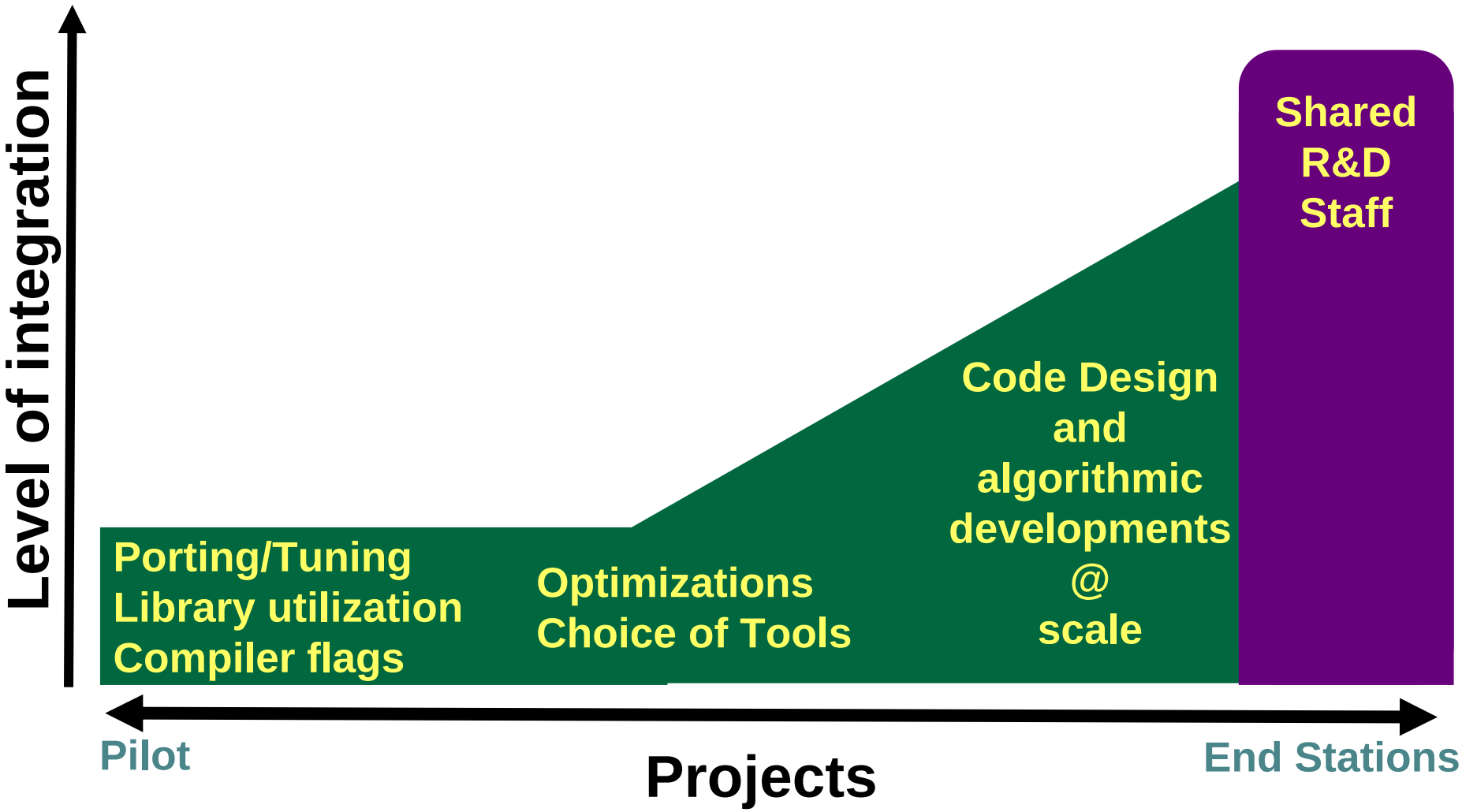


Whatever it Takes!

Scientific Computing Tasks and Deliverables

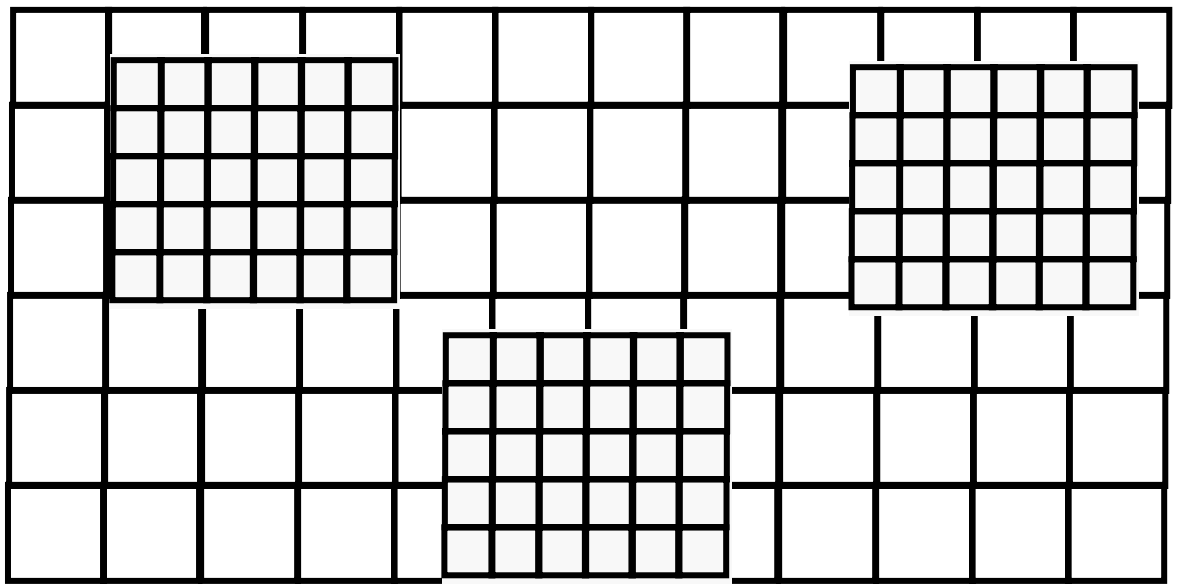
- **Project partnerships in science, visualization, workflow, and data analytics**
  - Level of integration is dependent upon the project
- **High-level user assistance**
  - Main staff function. Whatever it takes!
- **Algorithmic development at scale**
  - For scientific codes, visualization and workflow
- **Application and library code optimization and scaling**
  - How to use the LCF resources for science
- **User voice within LCF planning exercises**
  - Users are the focus.
- **Requirements gathering, documentation**
  - What's next for our users and our center
- **Exploiting parallel I/O & other technologies in applications**
  - Specific focus for targeted applications
- **Acquiring & deploying viz and end-to-end systems**
  - Infrastructure building and discovery.
- **Benchmarking and evaluation exercises with Vendor interaction**
  - Learning how to best use current and new LCF resources.

Partnership with Projects on LCF resources



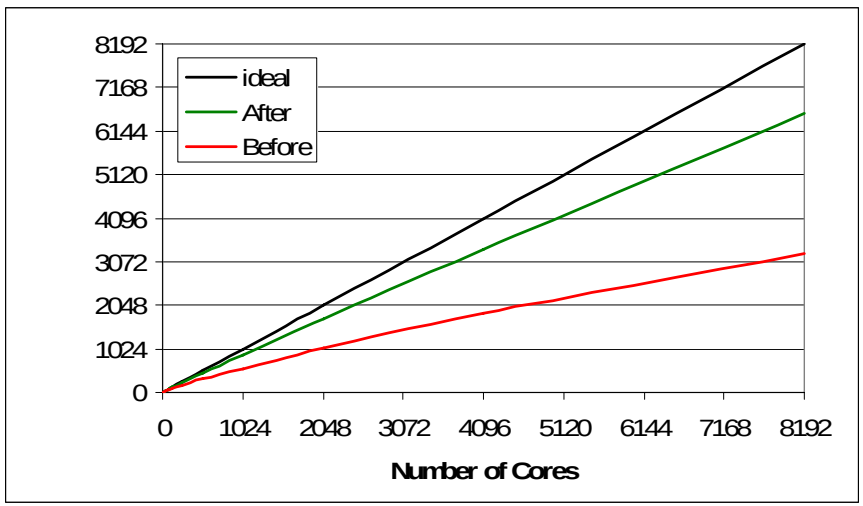
Algorithmic and programming model development at scale

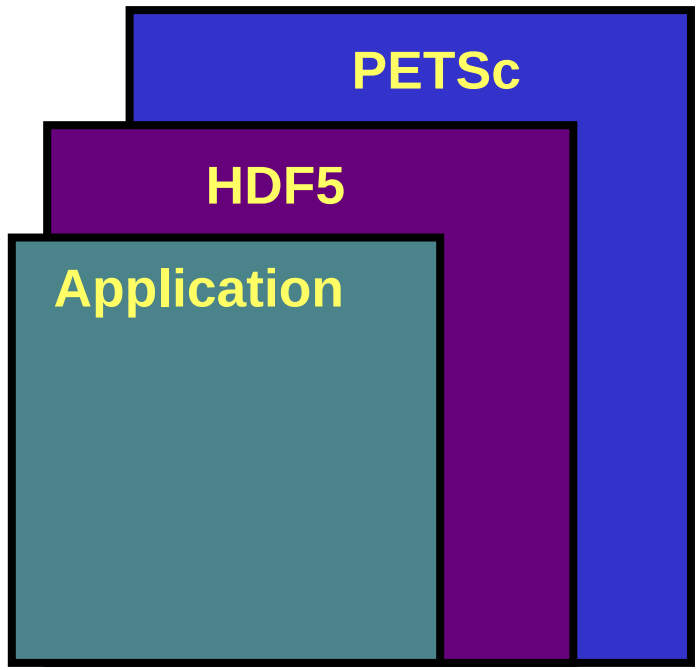
- **Complex Tradeoffs for applications**
  - Usually among storage, computation and communication
- **Redesign new methods**
  - Fixed grid to AMR grids
- **Programming model changes**
  - Message passing to one-sided model transformation



Application and Library Optimization and Scaling

- **Applications for the LCF systems**
  - Catamount issues for Apps
  - Dual Core/Single core settings
  - Compiler flags for optimal performance (Application/Library specific)
  - Modifications for scaling
- **Libraries Built and kept up-to-date**
  - HDF5, PETSc, FFTW, etc.





Requirements Gathering and Documentation

- **Participate in Applications Requirements Council (ARC)**
- **Determine requirements for applications on the machine**
  - Algorithmic
  - Programming models
  - Architectural
  - Infrastructure
- **Develop ties to applications areas not currently at scale on the machine**
  - Work with developers to understand application properties
    - Memory footprint
    - Algorithmic scalability
    - Potential for future resources

The Staff

- **Visualization**
  - Sean Ahern (Task Lead)
  - Ross Toedte
  - Jamison Daniel
  - George Ostrouchov
  - David Banks
- **End to End Solutions**
  - Scott Klasky (Task Lead)
  - Chen Jin
  - Roselyne Barreto








The Staff

- **Computational Science**
  - Richard Barrett
  - Mark Fahey
  - Ricky Kendall
  - Jeff Kuehn
  - Bronson Messer
  - Richard Mills
  - Arnold Tharrington
  - Trey White
  - Vickie Lynch
  - Sadaf Alam
  - Markus Eisenbach
  - Edo Apra
  - Ramanan Sankaran